

Toxic Release Stream Index for Inherently Safer Plant Design

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the

Chemical Engineering Department

Universiti Teknologi PETRONAS

In partial fulfilment of the requirement for the

Bachelor of Engineering (Hons)

(Chemical Engineering)

Approved by,

Dr Dzulkarnain Zaini

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained here have not been undertaken or done by unspecified sources or person.

.....

NIK ALHANA SABRINA BINTI NIK AMRI

ABSTRACT

An inherently safer design plant is one that avoids hazards instead of controlling them, particularly by reducing the amount of hazardous material and the number of hazardous operations in the plant. Since years before, plenty of researchers have developed methodologies and studies to enhance the implementation of inherent safety concept in the industry. Inherent safe is best when applied towards the preliminary stage of the design rather than towards the end, due to its ability to reduce the cost of the overall plant design. In conceptual design, process routes and streams can be compared and ranked by using inherent safety indices. Many indices has been developed but unable to cover all parameters of the inherent safety. This paper will focus on producing an index and implemented to evaluate the streams that are highly susceptible to loss of containment in the form of toxic release. A case study on Acrylic Acid production plant will then be used to evaluate the usage of the index developed by using the Toxic Release Stream Index (TRSI). The results presented towards the end of this work proves that the index produced may be able to point out the inherently unsafe streams and modify the design up to be acceptable level during the preliminary stage design stage.

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CHAPTER 1: INTRODUCTION

1.1 Background

Safety takes up a very crucial part of designing a process plant. Without proper focus on safety, major disasters due to chemical toxic release and explosions might happen, such as the Bhopal (1984) and Seveso (1976) disaster. In a typical process of designing any process plant, the safety approach usually is considered at the near end of the whole process. This leaves little to no space for safety issues to be avoided thus making the add-on enhancements the only option to reduce the hazard. Regular preventive maintenance plans are also added to the newly designed plant to reduce the risk of serious chemical accidents (Leong & Shariff, 2009). Control measures added late in design require continual staffing and maintenance throughout the life of the plant, greatly adding to the lifetime costs as well as repetitive training and documentation upkeep (Khan & Amyotte, 2002).

As said by Crowl and Louvar in 2002, a major accident is defined as “an unexpected, sudden occurrence such as a major emission, fire, or explosion resulting from uncontrolled developments in the course of the operation of any establishment and leading to serious danger to human health and/or the environment, immediate or delayed, inside or outside the establishment, and involving more dangerous substance”. Since the last few years, many new safety procedures introduced to evaluate hazards. However, accidents keep on happening because the available solutions do not minimize or eliminate them (Kletz, 1991).

The Seveso accident was a perfect example of a major accident regarding the release of toxic substances. The accident which happened in the year 1976 was a result of a failure in the overall reaction and causing the release of 6 tonnes of chemicals over an 18 kilometre squared area. Among the chemicals released was 1 kg of 2,3,7,8-tetrachlorodibenzodioxin (TCDD). High amount of TCDD resulted in few adverse effect ascertained such as chloracne (193 cases), peripheral neuropathy and liver enzyme induction (Bertazzi, 1991).

These accidents highlight the importance of safety as a step to prevent catastrophic events from happening. In addition to that, a lot of researches are trying to implement safety in the preliminary stage of the designing process so that the hazard can be reduced or eliminated thoroughly.

1.2 Problem Statement

Currently, the methods that are actively in used during the designing of any process plants are the ones that have been in used for a long time. The methods include Hazard and Operability Studies (HAZOP), DOW Fire and Explosion Index (DOW FEI), Quantitative Risk Assessment (QRA), et cetera. These methods involve doing hazard identification and also risk assessment and usually it is done towards the end of the design process. The alternative to this approach is to implement the inherent safety concept. This concept has been around for several years but it hasn't been widely used in the industry. In this approach, less reliance is placed on 'add-on' engineered safety systems and features, and procedural controls which can and do fail (Khan & Amyotte, 2005).

Many previous studies on inherent safety level (ISL) quantification index based are focusing on processing route. However, most of the work for index based inherent safety design (ISD) approach focusing on chemical route by using properties of single component. These indices lack of considering the chemical component as a mixture and developed purposely for toxic release.

Using a concept called Toxic Release Route Index (TRRI), the safest route can be obtained in a process design. After determining the safest route, the ISD can be applied at this stage by improving the inherent safety level of the streams. Further improvement can be done to ensure the ISD by ranking the process streams based on ISL within a process route. The selection of most hazardous streams can be done if the ISL of the process streams can be ranked through the technique such as the index based ISD approach. However, this concept has never been used for toxic release of the process streams.

1.3 Objectives and Scope of Study

The objectives of the project are:

- 1) To develop a new method of calculating the Toxic Release Stream Index based on the inherent safety concept
- 2) To implement the Toxic Release Stream Index to a case study to demonstrate its application in the industry
- 3) To compare the accuracy of results of toxic release between this paper and the previous researches

The scope of study includes:

- 1) Understanding the concept of inherent safety and its current application in the industry
- 2) Understanding the TRRI concept which gives a bigger picture in the TRSI
- 3) Using HYSYS to simulate the process stream in the process plant

The student is expected to understand the concept of inherent safety and the methodologies done by previous researches. Based on the recent studies, the student is expected to come up with an index which explains the possible toxic release of the streams in a process plant. This project aims to reduce the possibility of toxic release in a process stream by identifying them in the preliminary stage of the design.

CHAPTER 2: LITERATURE REVIEW

2.1 Inherent Safety

The inherent safety concept was first introduced by Trevor Kletz in his 1978 article entitled What You Don't Have, Can't Leak. The principles defining inherent safety as shown in Table 1 were formalized by Kletz (1991). Inherent safety focuses on avoiding hazards instead of controlling them, specifically by reducing the amount of hazardous material and the number of hazardous operations in the plant.

Table 1: Principles of inherent safety

Principles	Definition
Intensification	Reduction of the inventories of hazardous materials
Substitution	Change of hazardous chemicals substances by less hazardous chemicals
Attenuation	Reduction of the volumes of hazardous materials required in the process. Reduction of operation hazards by changing the processing conditions to lower temperatures, pressures or flows
Limitation of effects	The facilities must be designed in order to minimize effects of hazardous chemicals or energies releases
Simplification	Avoidance of complexities such as multi-product or multi-unit operations, or congested pipe or unit settings
Error tolerance	Making equipment robust, processes that can bear upsets, reactors able to withstand unwanted reactions, etc.

In any safety approach, the main aim is to minimize the total risk posed by a certain process plant. The risk is a product of the probability of an incident happening and the possible impact due to the incident actually happening. This is where inherent safety takes effect. Applying the principles to the inherent safety strategies themselves is obviously the most effective and straightforward approach, and has received the majority of attention in prior development of assessment tools (Heikkilä, 1999). However, the principles can also be applied at the other levels of the hierarchy, for

example leading to add-on measures that are more reliable, effective and thus making it inherently safer (Tugnoli, Khan, Amyotte, & Cozzani, 2008).

It is said that the possibility of implementing inherent safety decreases as the design proceeds (Rahman, Heikkilä, & Hurme, 2005) thus it is best to apply the IS concept in the preliminary design of the process plant. Based on the general principles in Table 1, a logical hierarchy of them are presented in Figure 1 below (Khan & Amyotte, 2002).

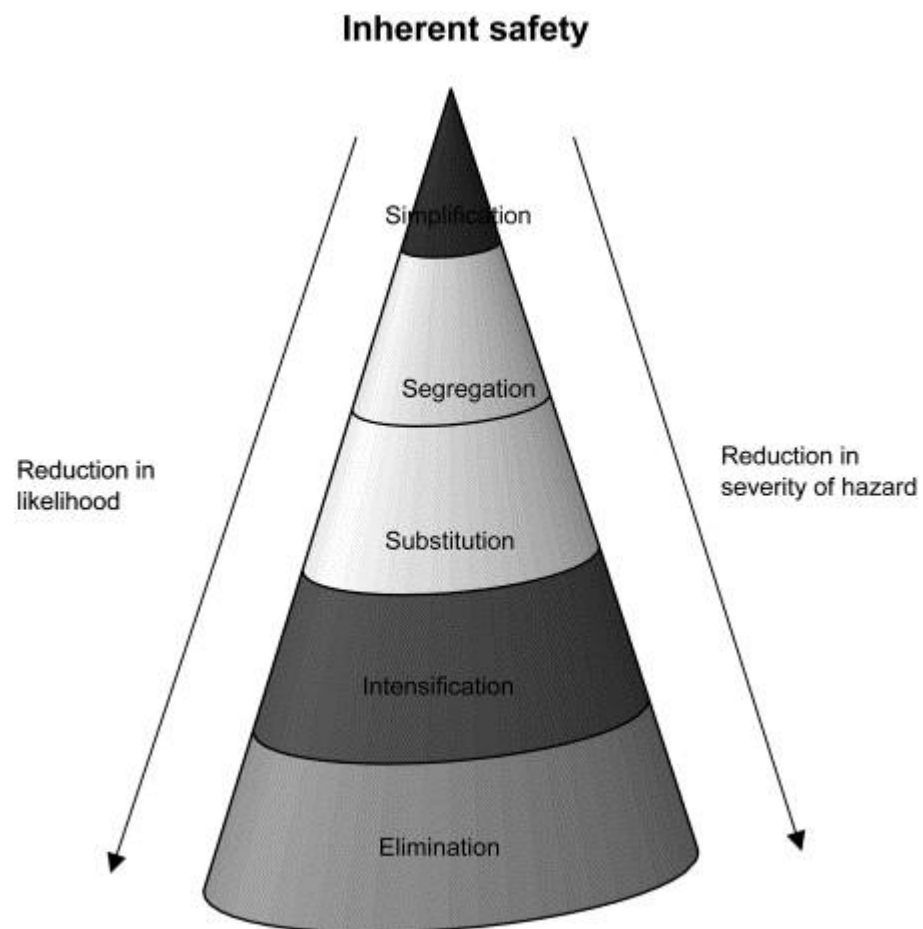


Figure 1: Hierarchy of the IS general principles

For example, the elimination or reduction in size of equipment can lead to the use of simpler, smaller, more compact equipment which offers the promise of reduced hazard and risks, reduced weight and space requirements, and less maintenance. In this way inherent safety approaches can provide the most cost-effective route to safety (Khan & Amyotte, 2002).

2.2 Previous Methodologies for Quantification on Inherent Safety Level

The evaluation methods of process safety have started from plenty of years back. Some of the methodologies were useful, but tedious to be implemented. Although the option of inherently safer design is economically viable, many researchers such as Kletz (1991), Moore et al., 2007 and Mansfield et al., 1966, Rushton et al. (1994), Moore (2007) had identified the lack of proper tool and system for its implementation as a key factor to poor application in the industry. Other than that, there is also a general lack of familiarity of the specific advantages of adopting an inherently safer approach to process design (Shariff, Leong, & Zaini, 2012). The other reasons for the lack of implementation of inherent safety are pictured in the figure 2 below (Kletz, 1991).

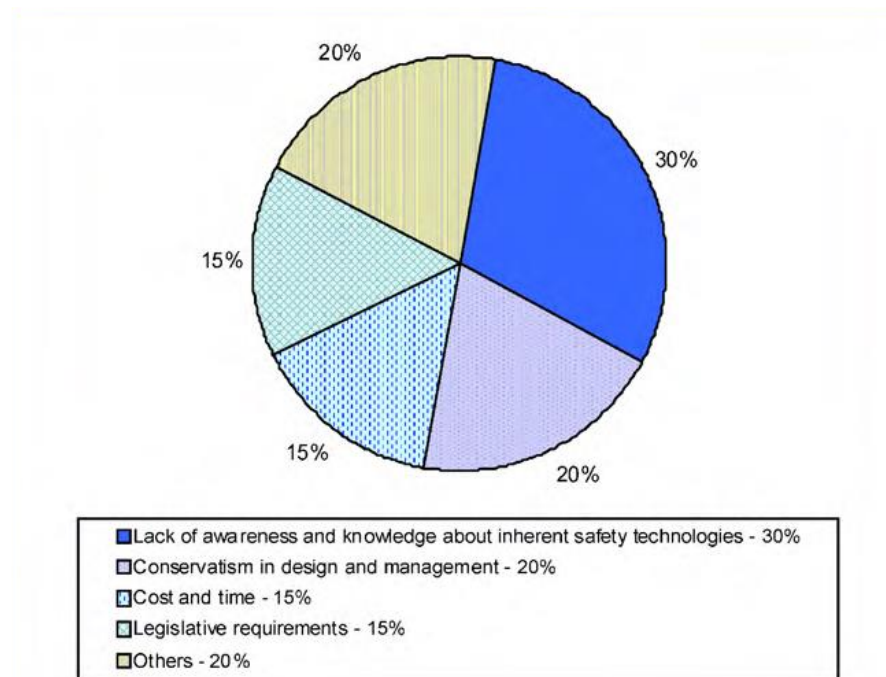


Figure 2: Problems of implementing inherent safety

In order to overcome the problems which was stated above, few researchers have proposed some methodologies for the assessment of the inherent safety level (ISL). One of the earliest methods proposed is the inherent safety checklist developed by Bollinger et al. (1996) and CCPS (1996). They provide extensive questions related to inherent safety and also provide guidance to implement inherent safety in process

design (Rusli & Mohd Shariff, 2010). The first published work was by Edwards and Lawrence in 1993 entitled “Prototype Index for Inherent Safety (PIIS)”. Basically, the indices for ranking alternatives chemical routes by Lawrence incorporated seven parameters relates to the physical properties of the chemicals and conditions of reaction steps which are, the temperature, pressure, reaction yield, inventory, toxicity, explosiveness and flammability. A trial inherent safety index has been developed for ranking alternative chemical routes by inherent safety. This index is later on implemented in a number of routes in produce methyl methacrylate (MMA). To verify and improve the index, a group of experts were asked to rank the routes and give comments on the new index developed. When compared, the new index matched with the experts ranking of the routes in the index. A new index has been created and from there, the process of improving the index will be repeated.

Next is the proposed Inherent Safety Index (ISI) methodology by Heikkila in 1999. Basically it is also an index developed to implement inherent safety in the early phases of design. The total index is divided into Chemical and Process Inherent Safety Index. The chemical inherent safety index is formed of sub-indices for reaction heats, flammability, explosiveness, toxicity, corrosiveness and chemical interaction. The process inherent safety index is formed of sub-indices for inventory, process temperature, pressure and the safety of equipment and process structure. When compared, Heikkila adapted a lot more parameters than Lawrence and Edwards but both still included toxic release as one of the parameters studied. The table below shows the summary of the parameters used by the two researchers.

Table 2: Parameters of inherent safety

	Edwards and Lawrence, (1993)	Heikkila (1999)
Inventory	x	x
Temperature	x	x
Pressure	x	x
Heat of main reaction	x	x
Heat of side reaction	-	x
Flammability	x	x
Explosiveness	x	x
Corrosiveness	-	x

Toxicity	x	x
Chemical interaction	-	x
Type of equipment	-	x
Safety of process structure	-	x

The following researchers focused to improve the indices such as i-Safe by Palaniappan (2002) while Gupta and Edwards (2003) developed a graphical method to measure ISL. Most of the ISL assessment methodologies that are proposed currently are focused on the indexing technique for process route evaluation. Khan and Amyotte (2005) proposed a method based on the word guide from HAZOP studies known as “integrated inherent safety index” (I2SI). The developed index was intended to be applied throughout the life cycle of process design.

The indices that are presently available mostly deal with a lot of data and it requires a tedious way of data transfer of process information and parameters for the inherent safety level calculation. This is then adapted by Mohd Shariff et al. (2006) to propose an integration of the process design simulator, HYSYS with the inherent safety index calculation by using the integrated risk estimation tool (iRET). The same concept was also picked up by Leong and Shariff (2008) in developing the inherent safety index module (ISIM) which integrates Microsoft Excel with HYSYS for simplicity of data transfer.

This paper aims to propose a new way of measuring the inherent safety level in process routes based on the toxic level of the stream. This concept is adapted from previous study on Process Stream Index (PSI) for explosiveness as a parameter done by Shariff, Leong and Zaini in 2012.

2.3 Toxic Release as Inherent Safety Parameter

2.3.1 Toxic Release Consequence Analysis Tool (TORCAT)

In a recent paper done by Mohd Shariff and Zaini in 2010, they developed a tool to properly analyse the inherent safety in plants, specifically on toxic release. This Toxic

Release Consequence Analysis Tool (TORCAT) framework allows them to detect which streams has the highest toxicity level evaluate them to ensure less to no harm will be done. This tool has an advantage from the others aforementioned in the sense that it directly links the software that is being used to simulate the process, iCON to an excel sheet where the results are displayed. The assessment tool was designed in a way that it could generate the outputs in the form of concentration level of toxic release and toxic effect from the source of release. This is as important as determining which stream that has the highest potential of toxic release as it is one of the mitigation tool used in the preliminary design stage. The framework for TORCAT is shown in the Figure 3 below.

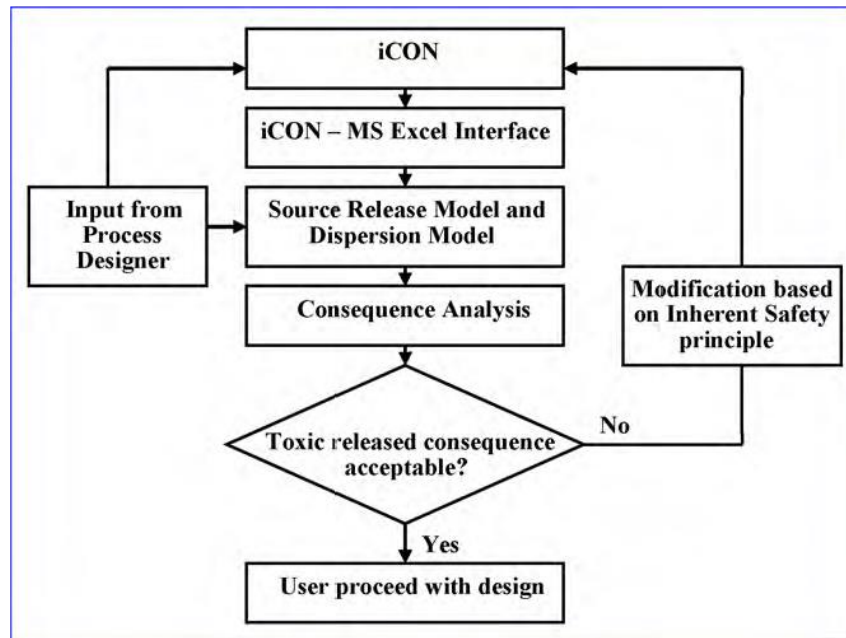


Figure 3: Framework for TORCAT

2.3.2 2-region Risk Matrix

In addition to that, in another paper done by Mohd Shariff and Zaini in 2013 also implement another method to assess the toxic release as inherent safety parameter. In this paper, they introduced a risk assessment concept to implement the inherent safety at the preliminary stage of the design. Their assessment is based on a 2-region matrix, which is also adapted from a previous study on explosion which reduce the risk to As Low as Reasonably Practical (ALARP). The design matrix is divided into 2 parts, acceptable and unacceptable. If the design condition falls into the unacceptable region,

the design can be improved by implementing the inherent safety principle to shift it towards the acceptable region. This approach aims to evaluate the risk of the process design thoroughly and also to identify the possible solution to eliminate or reduce the hazards, thus producing an inherently safer process design during the preliminary stage (Shariff & Zaini, 2013).

Likelihood of Occurrence (year ⁻¹)	Severity of Occurrence			Legend
	AEGL -1 [A] (ppm)	AEGL-2 [B] (ppm)	AEGL-3 [C] (ppm)	
Very High [1]	A1	B1	C1	Unacceptable
High [2]	A2	B2	C2	
Moderate [3]	A3	B3	C3	Acceptable
Low [4]	A4	B4	C4	
Very Low [5]	A5	B5	C5	
Unlikely [6]	A6	B6	C6	

Figure 4: 2-region risk matrix

2.3.3 Toxic Release Route Index (TRRI)

In a previous study done by Asari in 2014 shows that the toxic release route index (TRRI) is more inclined towards identifying the specific routes that is safest in a certain process. It is clear that there would be more than one route in a certain process and the index proves that it is valid by comparing it with several of the previous methodologies' results as well. The results from the study is shown in the table below. By knowing the route, the process designers can pay more attention to the safest route and apply the index that will be developed further in this paper that can identify streams with higher susceptibility to loss of containment. This concept is adapted from Process Route Index (PRI) done by Shariff and Leong which identifies the safest process route from explosion.

Table 3: Ranking of MMA process by various indices

Methyl Methacrylate Acid (MMA) process routes	Lawrence - PIIS	Expert Opinion	Heikkila - ISI	Leong & Shariff - PRI	TRRI
Ethylene via methyl propionate based route (C2/MP)	3	3	2	4	4
Ethylene via propionaldehyde based route (C2/PA)	4	4	3	3	3
Isobutylene based route (i-C4)	2	2	1	2	1
Tertiary Butyl Alcohol based route (TBA)	1	1	1	1	2

These papers study the same parameter of inherent safety which is the toxic release but from different point of view. Each and every study will contribute to inherent safety being widely used in the industry thus making accidents linking to toxic release prone to happen less. This paper behaves as a new method to determine which streams that need proper focus in case of a toxic release or loss of containment. The methodology for the index will be explained in the next chapter.

CHAPTER 3: METHODOLOGY/PROJECT WORK

3.1 Project Framework

This project aims to develop a new concept to quantify risk, which is inherent to the process plant at preliminary design stage. It is carried out by using an inherent risk assessment which is integrated with process design simulator to allow data transfer. A case study will be used to illustrate the advantage of implementing this technique. This project will be divided into 3 major stages. The 3 stages are explained as follows:

1) Initiation

This is the first stage of the project. During this stage, the student will analyse the streams and characterize the streams according to its pressure, density and toxicity level. The data can be found based on several sources. The pressure and density of the chemicals can be obtained through simulation software called HYSYS. For the purpose of determining the effect of chemicals used, the National Fire and Protection Agency (NFPA) 704 ranking value is chosen. NFPA 704 is a standard that is used to identify the hazards associated with materials. The NFPA 704 sets a hazard value ranging from 0 to 4 based on the ability of the chemical to cause any health hazard. The table below shows the description that fits for the NFPA 704 hazard values. This standard is chosen because it provides a simple and easily understood system of markings that can give a general idea of the hazards of the material and the severity of these hazards as they relate to emergency response.

This standard can be visually noticed by looking at the hazmat diamond. For each and every chemical, the diamond acts as a safety sign which shows user on the hazard of the chemical from the aspect of health hazard (blue), its flammability (red), reactivity (yellow) and any special hazard, if any (white).



Figure 5: Example of a hazmat diamond

Table 4: Standard System for the Identification of the Hazard Material for Emergency Response (NFPA 704, 2012)

Degrees of hazard	Criteria
0	Poses no health hazard, no precautions necessary and would offer no hazard beyond that of ordinary combustible materials
1	Exposure would cause irritation with only minor residual injury
2	Intense or continued but not chronic exposure could cause temporary incapacitation or possible residual injury
3	Short exposure could cause serious temporary or moderate residual injury
4	Very short exposure could cause death or major residual injury

Apart from using the NFPA standards, the Threshold Limit Values (TLV) could be another possible way to evaluate the toxicity level in a certain stream. This is due to its readily available data in most process industry. The standards on acceptable or tolerable risks are usually based on the risk statistics as well as the economy development level and the public value concept. Therefore the criteria are different from each other to some extent (Yu, Zhang, Wang, Ma, & Chen, 2009). For most chemicals, their respective TLVs can be located in the MSDS. TLV reflects a limit value of maximum exposure a worker can have without any adverse health effects. In this paper, the TLV for average exposure for a time of 8 hours per day is being used. It is important to use the same

threshold time for all TLV to ensure results are comparable. The table below shows the respective TLVs and its score.

Table 5: TLV values and respective scores

TLV range (ppm)	Score
TLV > 10000	0
TLV < 10000	1
TLV < 1000	2
TLV < 100	3
TLV < 10	4
TLV < 1	5
TLV < 0.1	6

As the TLV value increases, the score decreases. This means that the lower the score, the higher the toxicity level.

2) Calculation

This is the second stage of the project. The TRSI developed will serve as a numerical guideline of the overall safety of the stream for a plant. This project will take the assumption that the sudden loss of containment will happen instantaneously, releasing a huge amount of gas at the point of rupture. By taking the Gaussian Instantaneous Puff release model, the equation 3.1 below is produced.

$$\langle C \rangle(x, y, z, t) = \frac{Q_m^*}{\sqrt{2}(\pi)^{3/2} \sigma_x \sigma_y \sigma_z} \exp \left[-\frac{1}{2} \left(\left(\frac{x-ut}{\sigma_x} \right)^2 + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2} \right) \right] \quad \text{Eqn. 3.1}$$

Where

C is the time average concentration of centre puff cloud (kg/m³)

Q_m^* is the mass of material released (kg)

$\sigma_x \sigma_y \sigma_z$ are the dispersion coefficient in terms of x, y and z direction

(m)

x is the downwind direction (m)

y is the crosswind direction (m)
 z is the distance above the ground (m)
 t is the time since puff cloud release (s)

Based on the equation 3.1 above, the mass release is assumed to be an important parameter when dealing with toxic release. Apart from that, the toxicity level of the chemical at the point of release is equally important. The toxicity level of each stream is known during stage 1. The TRSI for each stream will be calculated by using the formula adapted from the PSI. This formula takes account the important variables that could affect the toxicity level of a certain stream.

$$TRSI = f(\text{mass release}, TL) \quad \text{Eqn. 3.2}$$

In a process stream, the toxicity level depends on the each chemical component present and the effects of each chemical to the stream. The presence of a chemical component in the stream will affect the overall toxicity of the stream. The term mass in the equation 3.2 above can be further converted to basic parameters using basic fluid dynamics properties. As said by Asari, the amount of mass flowing through in case of rupture is a function of density and pressure differential between the system and surrounding as per given in equation 3.3 below. The toxicity level is determined as the mass flow and the effect of the chemical NFPA 704 as described in Table 3.

$$\text{Toxicity level } (TL) = f(\text{mass flow avg}, \text{NFPA 704}) \quad \text{Eqn. 3.3}$$

The mass flow avg can be further explained by a combination of the mass flow with the mass fraction of the component in the stream.

$$TRSI = f(\text{pressure}, \text{density}, TL) \quad \text{Eqn. 3.4}$$

TRSI has a dimensionless unit, whereas the pressure and density have the unit of bar and kg/m³ respectively. The TRSI is then further evaluated by taking

the parameters individually and validating it against the average pressure, density and TL for each stream. This will give a suitable results that matches the overall toxicity of the plant.

$$I_p = \frac{\text{pressure value of individual stream}}{\text{average pressure of all streams}} \quad \text{Eqn 3.5}$$

$$I_\rho = \frac{\text{density value of individual stream}}{\text{average density of all streams}} \quad \text{Eqn. 3.6}$$

$$I_{TL} = \frac{\text{TL value of individual stream}}{\text{average TL of all streams}} \quad \text{Eqn. 3.7}$$

$$TRSI = A_o (I_p \times I_d \times I_{TL}) \quad \text{Eqn. 3.8}$$

Most of the indices developments are based on arbitrary decision. There is no single method to perform the indices exercise and the analyst can choose to develop their own numerical indices customized to their needs. For example the calculation of the Chemical Exposure Index (CEI) from Dow Chemical Company is a value of dimensionless arbitrarily defined numerical scale even though the parameters that contribute to the CEI are consisted unit measurements (CCPS, 1996). By following this previous indices experience, the TRSI is an arbitrarily average parameters combination calculations that influences the toxic release which is also dimensionless in value. Since the TRSI is to represent the overall process route index, the average value of parameters in equation 3.5, 3.6 and 3.7 are selected which results in equation 3.8. The empirical constant A_o is used to increase or decrease the magnitude of the resulting numbers for the calculation of TRSI. The value of A_o are depending on the units used and up to user to set its magnitude.

3) Comparison

This is the third stage. After the TRSI have been calculated, the values of each stream will be populated into a table and the higher the value of TRSI, the higher chance it has to a loss of containment. This concept provides a single

numerical value to represent the overall inherent safety level in a process stream. The ranking of the TRSI is mainly to alert the process designers to see which streams are more prone to danger and thus may opt to apply the inherent safety concept here by reducing the amount of hazardous materials used.

The results will then be compared to the previous study done by Shariff, Leong and Zaini in 2012 entitled Process Stream Index. This is done as a validation that the two parameters give results coherent with each other. To increase the strength of this validation, a correlation coefficient between the two parameters will be calculated. The formula that will be used is

$$r = \frac{n \sum xy - (\sum x)(\sum y)}{(n (\sum x^2) - (\sum x)^2)^{\frac{1}{2}} (n (\sum y^2) - (\sum y)^2)^{\frac{1}{2}}} \quad \text{Eqn 3.9}$$

The quantity r , called the linear correlation coefficient, measures the strength and the direction of a linear relationship between two variables.

Figure 6 shows the overview of the project.

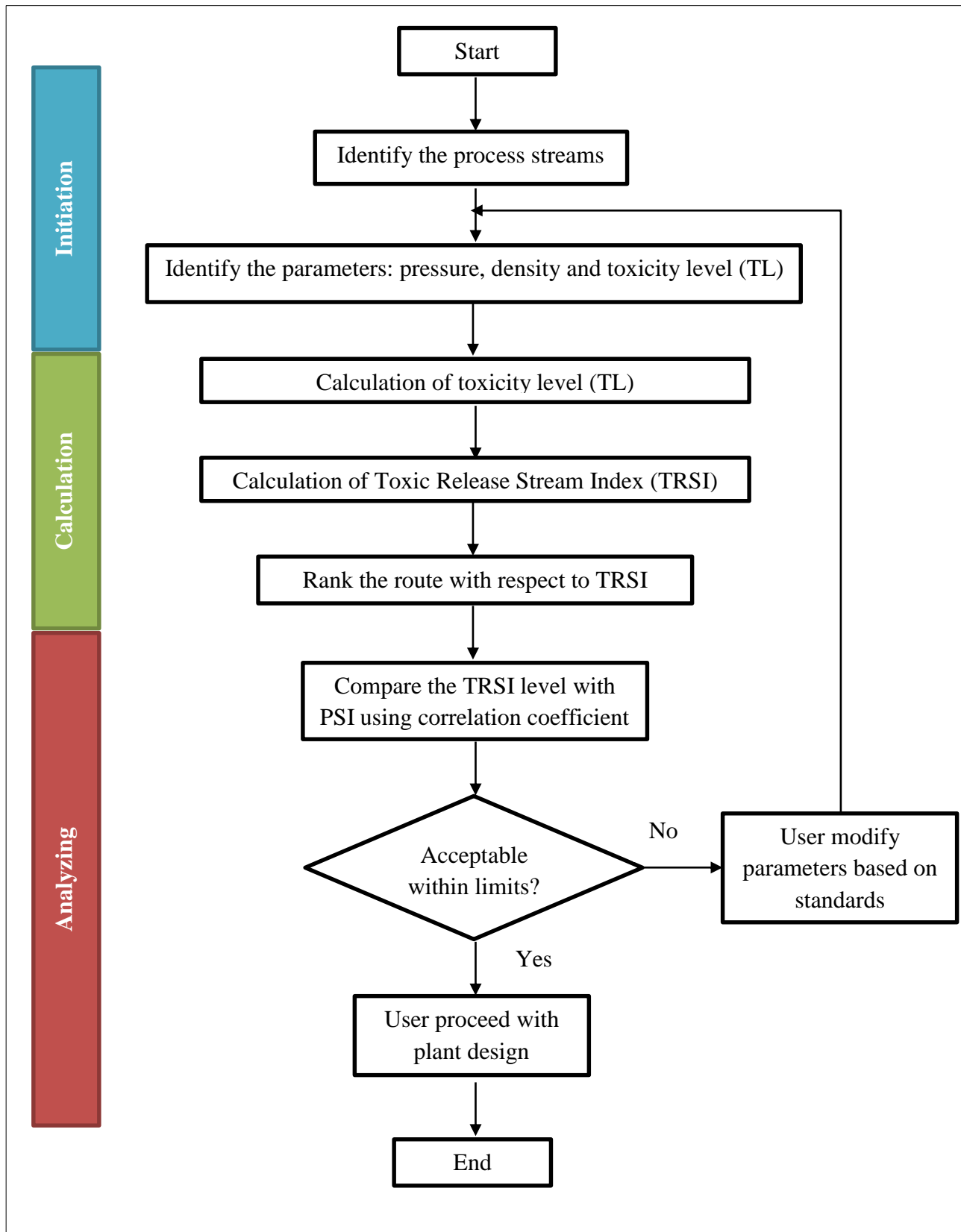


Figure 6: Flowchart of the proposed project

3.2 Gantt Chart

3.2.1 FYP I Timeline

Table 6: FYP I Gantt Chart

NO	Description\Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of Project Title														
2	Preliminary Research Work and Literature Review														
3	Submission of Extended Proposal														
4	Preparation for Proposal Defence														
5	Proposal Defence Presentation														
6	Continuation of Project Work														
7	Preparation of Interim Report														
8	Submission of Draft Interim Report														
9	Submission of Interim Final Report														

3.2.2 FYP II Timeline

Table 7: FYP II Gantt Chart

NO	Description\Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Identify case study														
2	Identify streams and chemicals used														
3	Calculation of toxicity level														
4	Calculation of TRSI														
5	Rank the streams according to TRSI and analyze														
6	Submission of progress report														
7	Preparation of poster and report														
8	Pre-SEDEX														
9	Submission of draft technical paper and dissertation														
10	Submission of technical paper														
11	Oral Presentation														
12	Submission of final Dissertation														

3.3 Case Study

To ensure the accuracy of the results, the TRSI will be studied using a readily available plant that can be improved using this index. The case study will be used to illustrate on how to prioritize streams according to its toxicity level. It is also demonstrated with the emphasis on application of inherent safety concept to eliminate or improve the consequence due to toxic release. The previous study on Toxic Release Route Index have been implemented to 4 different process routes to produce methyl methacrylate (MMA). This is due to the availability of previous methodologies done by Lawrence (2006) and Palaniappan (2002) thus making it easier to compare the accuracy of the results. For TRSI, the index will be implemented to an Acrylic Acid production plant developed by a previous study by Soo in 2004. The Figure 7 below will act as a base case for the case study. There are a total of 28 streams in the plant and TRSI will take account each streams as its own. The calculations and the index will be presented in the next chapter of the report which is in Results and Discussion.

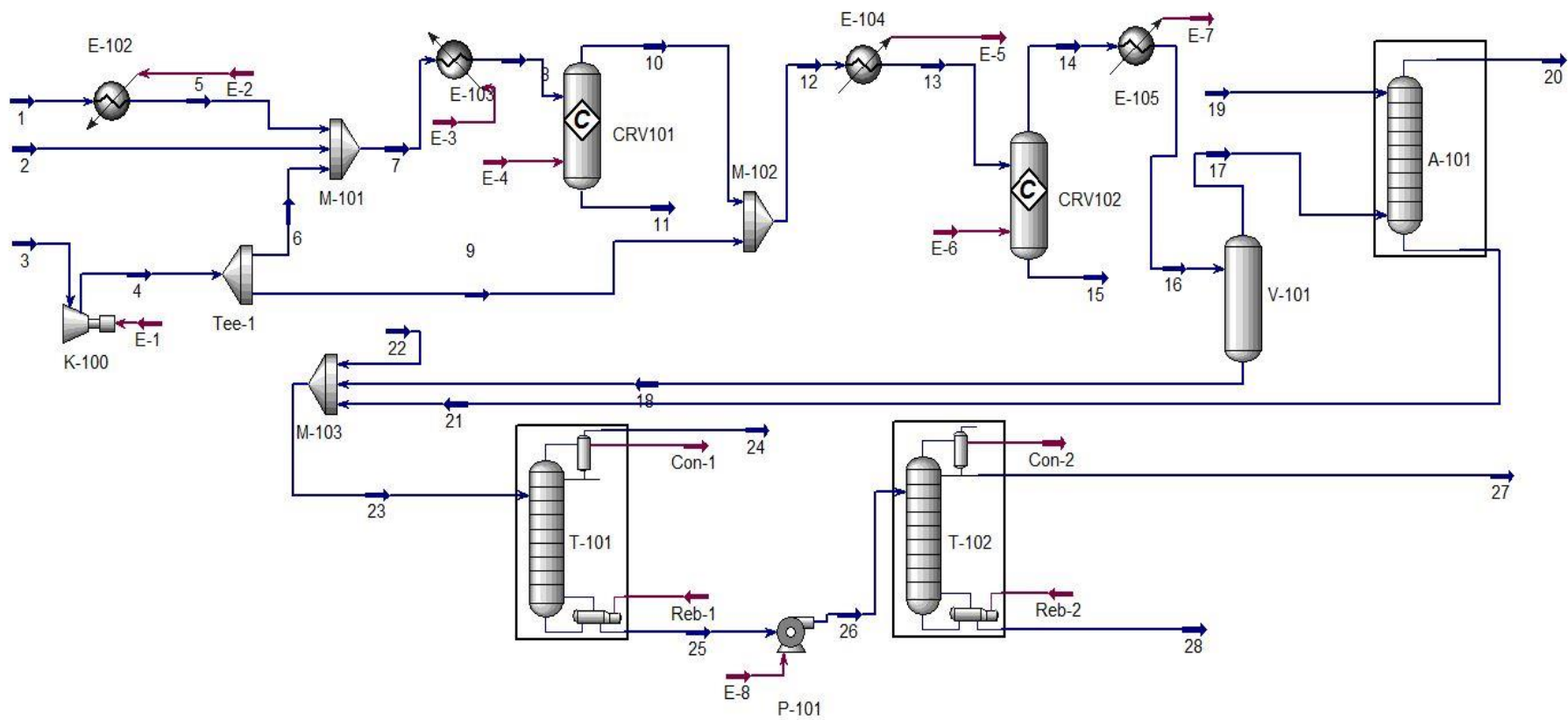


Figure 7: Acrylic Acid Production Plant base case study (Soo, 2004)

CHAPTER 4: RESULTS AND DISCUSSION

As mentioned above, the 3 parameters that are needed to calculate the TRSI are the pressure, density and the toxicity level of the streams (TL). These values can be obtained from the simulation of Acrylic Acid production via propylene oxidation. To compare between the parameters, each value will then be divided with the average value of the parameter for a given route. These are later than compiled and multiplied to calculate TRSI.

4.1 TRSI Results

Table 8: Pressure values of 28 streams

Stream	Pressure (bar)	Stream	Pressure (bar)	Stream	Pressure (bar)
1	2.5	11	2.5	21	1.3
2	5	12	2.5	22	2
3	1	13	2.5	23	1.3
4	2.5	14	2.5	24	0.025
5	2.5	15	2.5	25	0.043
6	2.5	16	2.5	26	0.5
7	2.5	17	2	27	0.09
8	2.5	18	2	28	0.11
9	2.5	19	2		
10	2.5	20	1.1		

Table 9: Relative ranking of I_p for 28 streams

Stream	I_p	Stream	I_p	Stream	I_p
1	1.30919	11	1.30919	21	0.68078
2	2.61839	12	1.30919	22	1.04736
3	0.52368	13	1.30919	23	0.68078
4	1.30919	14	1.30919	24	0.01309
5	1.30919	15	1.30919	25	0.02252
6	1.30919	16	1.30919	26	0.26184
7	1.30919	17	1.04736	27	0.04713
8	1.30919	18	1.04736	28	0.05760
9	1.30919	19	1.04736		
10	1.30919	20	0.57605		

By applying equation 3.4, a value of 1.9096 is obtained as the average pressure.

The I_p for stream 1 is 1.30919. This shows that stream 1 has 30.9% more pressure compared to the average pressure of all streams. When the I_p for all the streams are calculated and sorted from highest value to the lowest, it can be observed in Table 9 that stream 2 is relatively the highest in the rank of pressure. No initial evaluation can be made with only one parameter calculated thus it is also done for the other two parameters, namely density and TL. The calculation for the TL for each streams are as follows.

Table 10: TL calculation for 28 streams in Acrylic Acid Plant

Stream	1				2			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.20	0.000	3	0.000	4.40	0.000	3	0.000
Propane		0.052	2	0.126		0.000	2	0.000
Propene		0.948	1	1.142		0.000	1	0.000
Acrylic Acid		0.000	3	0.000		0.000	3	0.000
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.000	0	0.000		0.000	0	0.000
Oxygen		0.000	3	0.000		0.000	3	0.000
H2O		0.000	0	0.000		1.000	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				1.268				0.000

Stream	3				4			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	9.10	0.000	3	0.000	9.10	0.000	3	0.000
Propane		0.000	2	0.000		0.000	2	0.000
Propene		0.000	1	0.000		0.000	1	0.000
Acrylic Acid		0.000	3	0.000		0.000	3	0.000
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.767	0	0.000		0.767	0	0.000
Oxygen		0.233	3	6.356		0.233	3	6.356
H2O		0.000	0	0.000		0.000	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				6.356				6.356

Stream	5				6			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.20	0.000	3	0.000	5.59	0.000	3	0.000
Propane		0.052	2	0.126		0.000	2	0.000
Propene		0.948	1	1.142		0.000	1	0.000
Acrylic Acid		0.000	3	0.000		0.000	3	0.000
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.000	0	0.000		0.767	0	0.000
Oxygen		0.000	3	0.000		0.233	3	3.907
H2O		0.000	0	0.000		0.000	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				1.268				3.907

Stream	7				8			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	11.19	0.000	3	0.000	11.19	0.000	3	0.000
Propane		0.006	2	0.126		0.006	2	0.126
Propene		0.102	1	1.142		0.102	1	1.142
Acrylic Acid		0.000	3	0.000		0.000	3	0.000
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.383	0	0.000		0.383	0	0.000
Oxygen		0.116	3	3.907		0.116	3	3.907
H2O		0.393	0	0.000		0.393	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				5.174				5.174

Stream	9				10			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	3.51	0.000	3	0.000	11.19	0.012	3	0.396
Propane		0.000	2	0.000		0.006	2	0.126
Propene		0.000	1	0.000		0.003	1	0.034
Acrylic Acid		0.000	3	0.000		0.010	3	0.341
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.119	4	5.323
Nitrogen		0.767	0	0.000		0.383	0	0.000
Oxygen		0.233	3	2.450		0.029	3	0.969
H2O		0.000	0	0.000		0.439	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				2.450				7.189

Stream	11				12			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	0.00	0.044	3	0.000	14.70	0.009	3	0.396
Propane		0.000	2	0.000		0.004	2	0.126
Propene		0.000	1	0.000		0.002	1	0.034
Acrylic Acid		0.006	3	0.000		0.008	3	0.341
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.023	4	0.000		0.091	4	5.323
Nitrogen		0.091	0	0.000		0.475	0	0.000
Oxygen		0.005	3	0.000		0.078	3	3.418
H2O		0.832	0	0.000		0.334	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				0.000				9.639

Stream	13				14			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	14.70	0.009	3	0.396	14.70	0.013	3	0.553
Propane		0.004	2	0.126		0.004	2	0.126
Propene		0.002	1	0.034		0.002	1	0.034
Acrylic Acid		0.008	3	0.341		0.119	3	5.268
Acetic Acid		0.000	3	0.000		0.002	3	0.086
Acrolein		0.091	4	5.323		0.001	4	0.053
Nitrogen		0.475	0	0.000		0.475	0	0.000
Oxygen		0.078	3	3.418		0.049	3	2.176
H2O		0.334	0	0.000		0.335	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				9.639				8.296

Stream	15				16			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	0.00	0.008	3	0.000	14.70	0.013	3	0.553
Propane		0.000	2	0.000		0.004	2	0.126
Propene		0.000	1	0.000		0.002	1	0.034
Acrylic Acid		0.337	3	0.000		0.119	3	5.268
Acetic Acid		0.006	3	0.000		0.002	3	0.086
Acrolein		0.001	4	0.000		0.001	4	0.053
Nitrogen		0.009	0	0.000		0.475	0	0.000
Oxygen		0.001	3	0.000		0.049	3	2.176
H2O		0.639	0	0.000		0.335	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				0.000				8.296

Stream	17				18			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	9.09	0.020	3	0.551	5.61	0.000	3	0.002
Propane		0.007	2	0.126		0.000	2	0.000
Propene		0.004	1	0.034		0.000	1	0.000
Acrylic Acid		0.011	3	0.312		0.295	3	4.955
Acetic Acid		0.000	3	0.013		0.004	3	0.073
Acrolein		0.001	4	0.038		0.001	4	0.016
Nitrogen		0.767	0	0.000		0.000	0	0.000
Oxygen		0.080	3	2.176		0.000	3	0.000
H2O		0.109	0	0.000		0.700	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				3.249				5.047

Stream	19				20			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.05	0.000	3	0.000	8.98	0.020	3	0.551
Propane		0.000	2	0.000		0.007	2	0.126
Propene		0.000	1	0.000		0.004	1	0.034
Acrylic Acid		0.000	3	0.000		0.001	3	0.015
Acetic Acid		0.000	3	0.000		0.000	3	0.002
Acrolein		0.000	4	0.000		0.001	4	0.036
Nitrogen		0.000	0	0.000		0.777	0	0.000
Oxygen		0.000	3	0.000		0.081	3	2.176
H2O		1.000	0	0.000		0.110	0	0.000
Hydroquinone		0.000	2	0.000		0.000	2	0.000
				0.000				2.940

Stream	21				22			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.16	0.000	3	0.000	0.01	0.000	3	0.000
Propane		0.000	2	0.000		0.000	2	0.000
Propene		0.000	1	0.000		0.000	1	0.000
Acrylic Acid		0.085	3	0.297		0.000	3	0.000
Acetic Acid		0.003	3	0.011		0.000	3	0.000
Acrolein		0.000	4	0.001		0.000	4	0.000
Nitrogen		0.000	0	0.000		0.000	0	0.000
Oxygen		0.000	3	0.000		0.000	3	0.000
H2O		0.911	0	0.000		0.000	0	0.000
Hydroquinone		0.000	2	0.000		1.000	2	0.015
				0.309				0.015

Stream	23				24			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	6.78	0.000	3	0.002	5.02	0.000	3	0.002
Propane		0.000	2	0.000		0.000	2	0.000
Propene		0.000	1	0.000		0.000	1	0.000
Acrylic Acid		0.258	3	5.253		0.001	3	0.011
Acetic Acid		0.004	3	0.084		0.006	3	0.084
Acrolein		0.001	4	0.017		0.001	4	0.017
Nitrogen		0.000	0	0.000		0.000	0	0.000
Oxygen		0.000	3	0.000		0.000	3	0.000
H2O		0.736	0	0.000		0.993	0	0.000
Hydroquinone		0.001	2	0.015		0.000	2	0.000
				5.371				0.114

Stream	25				26			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.76	0.000	3	0.000	1.76	0.000	3	0.000
Propane		0.000	2	0.000		0.000	2	0.000
Propene		0.000	1	0.000		0.000	1	0.000
Acrylic Acid		0.995	3	5.242		0.995	3	5.242
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.000	0	0.000		0.000	0	0.000
Oxygen		0.000	3	0.000		0.000	3	0.000
H2O		0.000	0	0.000		0.000	0	0.000
Hydroquinone		0.004	2	0.015		0.004	2	0.015
				5.257				5.257

Stream	27				28			
Material	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL	Mass Flow (kg/s)	Mass Fraction	NFPA 704	TL
CO2	1.74	0.000	3	0.000	0.02	0.000	3	0.000
Propane		0.000	2	0.000		0.000	2	0.000
Propene		0.000	1	0.000		0.000	1	0.000
Acrylic Acid		1.000	3	5.213		0.556	3	0.029
Acetic Acid		0.000	3	0.000		0.000	3	0.000
Acrolein		0.000	4	0.000		0.000	4	0.000
Nitrogen		0.000	0	0.000		0.000	0	0.000
Oxygen		0.000	3	0.000		0.000	3	0.000
H2O		0.000	0	0.000		0.000	0	0.000
Hydroquinone		0.000	2	0.000		0.444	2	0.015
				5.213				0.044

Following the calculation of the TL, the I_{TL} for each stream is then calculated using equation 3.6. A value of 3.8510 is obtained as the average TL. The I_{TL} for stream 1 is 1.2677. This shows that stream 1 has 26.7% more TL value compared to the average pressure of all streams. The tabulated I_{TL} is shown in table below.

Table 11: Relative ranking of I_{TL} for 28 streams

Stream	I_{TL}	Stream	I_{TL}	Stream	I_{TL}
1	0.3292	11	0.0000	21	0.0803
2	0.0000	12	2.5029	22	0.0040
3	1.6505	13	2.5029	23	1.3948
4	1.6505	14	2.1542	24	0.0297
5	0.3292	15	0.0000	25	1.3651
6	1.0145	16	2.1542	26	1.3651
7	1.3436	17	0.8437	27	1.3537
8	1.3436	18	1.3105	28	0.0114
9	0.6361	19	0.0000		
10	1.8669	20	0.7633		

The result is a relative ranking of all the stream within all the streams in a process route portrayed in Table 12 below, as explained in section 3.1, (2). The resulting dimensionless numbers can be used to clearly differentiate the streams when considering the parameters individually. The primary function of these numbers is to give an index that reflects the severity of the process stream in a case of toxic release or loss of containment. It is to be noted that the higher the value of TRSI, the less inherently safe the plant is. By using this index, it is possible to identify and eliminate the most inherently unsafe at the preliminary design stage of the process plant. It can also help to eliminate other streams will zero value as the streams will not cause any hazard based on this index. Its validity will be discussed further in the next section.

Table 12: Relative Ranking of TRSI for 28 streams

Stream	I_p	I_ρ	I_{TL}	TRSI
18	1.04736	2.4125	1.3105	49.67
23	0.68078	2.3748	1.3948	33.82
26	0.26184	2.4780	1.3651	13.29
27	0.04713	2.4330	1.3537	2.33
21	0.68078	2.4177	0.0803	1.98
25	0.02252	2.4780	1.3651	1.14
16	1.30919	0.0095	2.1542	0.40
13	1.30919	0.0035	2.5029	0.17
4	1.30919	0.0051	1.6505	0.16
14	1.30919	0.0038	2.1542	0.16
12	1.30919	0.0033	2.5029	0.16
22	1.04736	2.4160	0.0040	0.15
10	1.30919	0.0030	1.8669	0.11
7	1.30919	0.0041	1.3436	0.11
6	1.30919	0.0051	1.0145	0.10
1	1.30919	0.0127	0.3292	0.08
8	1.30919	0.0030	1.3436	0.08
9	1.30919	0.0051	0.6361	0.06
5	1.30919	0.0094	0.3292	0.06
17	1.04736	0.0036	0.8437	0.05
3	0.52368	0.0028	1.6505	0.04
28	0.05760	2.3731	0.0114	0.02
20	0.57605	0.0027	0.7633	0.02
24	0.01309	0.0000	0.0297	0.00
2	2.61839	0.0057	0.0000	0.00
11	1.30919	2.6853	0.0000	0.00
15	1.30919	3.3640	0.0000	0.00
19	1.04736	2.4854	0.0000	0.00

Based on Table 12, streams 18, 23 and 26 shows the highest values as opposed to streams 24, 2, 11, 15 and 19 which shows 0. When analysing the chance of toxic release in the plant, streams with zero value can be eliminated completely while the major streams with high value of TRSI are the ones that needs to be looked out for.

4.2 Comparison of TRSI with Process Stream Index (PSI)

The Acrylic Acid production plant HYSYS simulation (Soo, 2008) has been tested by two different indexes, one done by Shariff et al. (2012) and the other one in this project. Both study uses similar methodology to calculate the index in which both of them takes the ratio of a particular parameter for the selected stream against the average value of the parameters that are involved. The results from this two study are presented in Table 13, in which the PSI results are in the middle column and TRSI in the most left column. It can be concluded from the results that both of the index show stream 18 being the most inherently unsafe by having the highest score among 28 streams calculated from the perspective of explosiveness (PSI) and toxic release (TRSI). Thus, both the PSI and TRSI are examples of indexes that are developed to reflect the degree of hazard that is inherent to the design and have the ability to account for the properties inside the mixture instead of as an individual component to quantify the inherent safety level (ISL).

To check that both of the index are linear with each other, the data set from the Table 12 can be numerically represented by a correlation coefficient. The formula is given in Section 3.1 (3) above. The correlation coefficient measures the strength and direction of a linear relationship between the two sets of data. The correlation coefficient for this study is calculated both manually and by using PEARSON function (Statistic 2, 2011) which follows closely with the methodology of Shariff et al. (2012).

Table 13: Inherent safety indices for Acrylic Acid production plant streams

	Process stream Index (PSI) (Shariff et al., 2012)	Toxic Release Stream Index (TRSI)
Acrylic Acid Stream (Soo, 2004)	Calculated value	Calculate value
1	0.11	0.08
2	0.00	0.00
3	0.00	0.04
4	0.08	0.16
5	0.00	0.06
6	0.08	0.10
7	0.05	0.11
8	0.05	0.08
9	0.00	0.06
10	0.12	0.11
11	0.00	0.00
12	0.12	0.16
13	0.13	0.17
14	0.04	0.16
15	0.00	0.00
16	0.09	0.40
17	0.00	0.05
18	13.54	49.67
19	0.00	0.00
20	0.00	0.02
21	0.00	1.98
22	0.00	0.15
23	12.52	33.82
24	0.00	0.00
25	0.10	1.14
26	1.16	13.29
27	0.20	2.33
28	0.44	0.02

Based on the formula, the value of r can be $-1 < r < +1$. The + and – signs are used for positive linear correlations and negative linear correlations, respectively. The results of this coefficient can be divided into 4 groups namely:

1) Positive correlation

If x and y have a strong positive linear correlation, r is close to $+1$. An r value of exactly $+1$ indicates a perfect positive fit. Positive values indicate a directly proportional relationship between x and y variables. It is such that if x increase, y will also increase.

2) Negative correlation

If x and y have a strong negative linear correlation, r is close to -1 . An r value of exactly -1 indicates a perfect negative fit. Positive values indicate an inversely proportional relationship between x and y variables. It is such that if x increase, y will decrease.

3) No correlation

If there is no linear correlation or a weak linear correlation, r is close to zero. A value near zero means that there is a random nonlinear relationship between the variable x and y . Note that r is a dimensionless quantity, thus it does not depend on the units involved.

4) A perfect correlation

This is a special case where it only occurs if all of the data points lie exactly on a straight line. If $r = +1$, the slope of this line is positive. If $r = -1$, the slope of this line is negative.

A correlation with coefficient that is greater than 0.8 is generally described as strong, while a correlation less than 0.5 is generally described as weak. The calculation is laid out in the Table 14 below.

Table 14: Correlation Coefficient between TRSI and PSI

	STREAM	TRSI (x)	PSI (y)	n	x	x^2	y	y^2	xy
1	18	49.7	13.5	1	49.7	2467.1	13.5	182.3	670.5
2	23	33.8	12.4	2	33.8	1144.1	12.4	153.8	419.4
3	26	13.3	1.2	3	13.3	176.5	1.2	1.4	15.9
4	27	2.3	0.2	4	2.3	5.4	0.2	0.0	0.5
5	21	2.0	0	5	2.0	3.9	0	0.0	0.0
6	25	1.1	0.1	6	1.1	1.3	0.1	0.0	0.1
7	16	0.4	0.1	7	0.4	0.2	0.1	0.0	0.0
8	13	0.2	0	8	0.2	0.0	0	0.0	0.0
9	4	0.2	0	9	0.2	0.0	0	0.0	0.0
10	14	0.2	0.2	10	0.2	0.0	0.2	0.0	0.0
11	12	0.2	0.1	11	0.2	0.0	0.1	0.0	0.0
12	22	0.2	0.1	12	0.2	0.0	0.1	0.0	0.0
13	10	0.1	0.1	13	0.1	0.0	0.1	0.0	0.0
14	7	0.1	0.1	14	0.1	0.0	0.1	0.0	0.0
15	6	0.1	0.1	15	0.1	0.0	0.1	0.0	0.0
16	1	0.1	0.5	16	0.1	0.0	0.5	0.3	0.0
17	8	0.1	0.1	17	0.1	0.0	0.1	0.0	0.0
18	9	0.1	0	18	0.1	0.0	0	0.0	0.0
19	5	0.1	0	19	0.1	0.0	0	0.0	0.0
20	17	0.0	0	20	0.0	0.0	0	0.0	0.0
21	3	0.0	0	21	0.0	0.0	0	0.0	0.0
22	28	0.0	0	22	0.0	0.0	0	0.0	0.0
23	20	0.0	0	23	0.0	0.0	0	0.0	0.0
24	24	0.0	0	24	0.0	0.0	0	0.0	0.0
25	2	0.0	0	25	0.0	0.0	0	0.0	0.0
26	11	0.0	0	26	0.0	0.0	0	0.0	0.0
27	15	0.0	0	27	0.0	0.0	0	0.0	0.0
28	19	0.0	0	28	0.0	0.0	0	0.0	0.0
					104.2	3798.8	28.8	337.9	1106.7

$$n = 28$$

$$\Sigma x = 104.2$$

$$\Sigma y = 28.8$$

$$\Sigma x^2 = 3798.8$$

$$\Sigma y^2 = 337.9$$

$$\Sigma xy = 1106.7$$

$$r = 0.97$$

4.3 Mitigation Action

To reduce the severity of the streams that has high values of TRSI, author has come up with a mitigation plan since the index is at the preliminary design stage. Some of the options considered are reducing the number of equipments used, reducing the amount of hazardous material used or changing the parameters used in the process stream. All of the options follow closely the criterias that was aligned by Kletz which are shown in Table 1. The user can also apply other methodologies such as TORCAT to calculate the significant difference by using probit analysis to determine the before and after consequences of the reduced value of TRSI.

The objective is to change the parameters without affecting the products at the end of the process stream. By altering the pressure, the amount of Acrylic Acid produced can still be maintained while the probability of streams 18, 23 and 26 to have a toxic release are decreased. By reducing the pressures of entering components in Streams 1 and 2 by half, it can make a huge difference in the TRSI value of process. The table below shows the altered values of pressure for the process.

Table 15: Altered values of pressure for 28 streams

Stream	I_{TL}	Stream	I_{TL}	Stream	I_{TL}
1	1	11	2.5	21	1.3
2	2.5	12	2.5	22	1
3	1	13	2.5	23	1
4	2.5	14	2.5	24	0.025
5	2.5	15	2.5	25	0.043
6	2.5	16	2.5	26	0.1
7	2.5	17	1.5	27	0.09
8	2.5	18	1.5	28	0.11
9	2.5	19	2		
10	2.5	20	1.1		

These changed values of pressure will result in a change of TRSI values of:

Stream 18: 49.67 to 42.59

Stream 23: 33.82 to 29.75

Stream 26: 13.29 to 3.04

The changes in pressure can contribute to reduce of up to 23% in the TRSI value.

CHAPTER 5: CONCLUSION AND RECOMMENDATION

As a conclusion, Inherent Safety Level quantification remains as one of the important factor in the challenge for inherent safety concept to gain industry acceptance. Few pioneering indices to quantify inherent safety have been proposed in the past. These indices though are moderately simple to use, still have many rooms for improvement in order to represent the process stream condition more accurately. An inherent safety option may not always be the best option due to the possibility that it might be costly or not feasible within the project timetable compared to trusted additions measures. Rather, the aim of inherent safety is to encourage designers to integrate safety with design and to tackle safety issues at the earliest stage possible. This paper will allow the designers to focus on the specific streams to prevent any toxic release leading to any catastrophic event from happening. It demonstrated the importance to have a quantitative method to measure the toxicity level of each stream in a process plant.

The case study which implemented the index at a preliminary stage proves to be an effective test as it produces a satisfactory result for this level. The index's validity enhances as the TRSI produced are parallel to the PSI on the streams that are the most inherently unsafe. A method have been introduced to reduce the value of TRSI in order to reduce the hazard up to 23%. It is believed that there are potential for future work in expanding this project by introducing other parameters to further enhance the validity of this index.

CHAPTER 6: REFERENCES

- Asari, S. (2014). Toxic Release Route index for inherently safer plant design, Bachelor Engineering Final Year Plant Design Project, Universiti Teknologi PETRONAS, Malaysia
- Bertazzi, P. A. (1991). Long-term effects of chemical disasters. Lessons and results from Seveso. *Science of The Total Environment*, 106(1–2), 5-20. doi: [http://dx.doi.org/10.1016/0048-9697\(91\)90016-8](http://dx.doi.org/10.1016/0048-9697(91)90016-8)
- Crowl, D. A. And Louvar J. F., (2002) Chemical Process Safety: Fundamentals with Applications, Prentice Hall, Eaglewood Cliffs, N. J.
- Heikkilä, A.M., (1999). Inherent Safety in Process Plant Design, Ph.D. Thesis, VTT Publication Number 384, Helsinki University of Technology, Espoo, Finland.
- Khan, F. I., & Amyotte, P. R. (2002). Inherent safety in offshore oil and gas activities: a review of the present status and future directions. *Journal of Loss Prevention in the Process Industries*, 15(4), 279-289. doi: [http://dx.doi.org/10.1016/S0950-4230\(02\)00009-8](http://dx.doi.org/10.1016/S0950-4230(02)00009-8)
- Khan, F. I., & Amyotte, P. R. (2005). I2SI: A comprehensive quantitative tool for inherent safety and cost evaluation. *Journal of Loss Prevention in the Process Industries*, 18(4–6), 310-326. doi: <http://dx.doi.org/10.1016/j.jlp.2005.06.022>
- Lawrence, D., 1996. Quantifying Inherent Safety of Chemical Process Routes, Ph.D. Thesis, Loughborough University, Loughborough, UK,
- Leong, C. T., & Shariff, A. M. (2009). Process route index (PRI) to assess level of explosiveness for inherent safety quantification. *Journal of Loss Prevention in the Process Industries*, 22(2), 216-221. doi: <http://dx.doi.org/10.1016/j.jlp.2008.12.008>

- Mansfield, D.P., Kletz, T.A., Al-Hassan, T., 1996. Optimizing safety by inherent offshore platform design. In: Proceedings of the 1st International Conference on Health, Safety and Environment, The Hague, The Netherlands.
- Moore, D.A., Hazzan, M., Rose, M., Heller, D., Hendershot, C.D., Dowell III et al., 2007. Advances in inherent safety guidance. *Process Safety Progress* 27 (June (2)) 115-120.
- NFPA 704 (2012) http://en.wikipedia.org/wiki/NFPA_704. Accessed on 25.02.2015
- Palaniappan, C., (2002). Expert System for Design of Inherently Safer Chemical Processes, M. Eng. Thesis, National University of Singapore, Singapore.
- Rahman, M., Heikkilä, A.-M., & Hurme, M. (2005). Comparison of inherent safety indices in process concept evaluation. *Journal of Loss Prevention in the Process Industries*, 18(4–6), 327-334. doi: <http://dx.doi.org/10.1016/j.jlp.2005.06.015>
- Rusli, R., & Mohd Shariff, A. (2010). Qualitative Assessment for Inherently Safer Design (QAISD) at preliminary design stage. *Journal of Loss Prevention in the Process Industries*, 23(1), 157-165. doi: <http://dx.doi.org/10.1016/j.jlp.2009.07.005>
- Shariff, A.M., Zaini, D. (2010). "Toxic Release Consequence Analysis Tool (TORCAT) for inherently safer design plant", *Journal of Hazardous Materials* 182, 394-402, Elsevier Science Ltd
- Shariff, A. M., Leong, C. T., & Zaini, D. (2012). Using process stream index (PSI) to assess inherent safety level during preliminary design stage. *Safety Science*, 50(4), 1098-1103. doi: <http://dx.doi.org/10.1016/j.ssci.2011.11.015>
- Shariff, A. M., & Zaini, D. (2013). Inherent risk assessment methodology in preliminary design stage: A case study for toxic release. *Journal of Loss*

Prevention in the Process Industries, 26(4), 605-613. doi:
<http://dx.doi.org/10.1016/j.jlp.2012.12.003>

Soo, E.W., (2004) Acrylic Acid Production Plant, Bachelor Engineering Final Year
Plant Design Project, Universiti Teknologi PETRONAS, Malaysia

Statistic 2, (2011) <
<http://mathbits.com/MathBits/TISection/Statistics2/correlation.htm>>.
Accessed on 03.02.2015

Tugnoli, A., Khan, F., Amyotte, P., & Cozzani, V. (2008). Safety assessment in plant
layout design using indexing approach: Implementing inherent safety
perspective: Part 1 – Guideword applicability and method description. *J
Hazard Mater*, 160(1), 100-109. doi:
<http://dx.doi.org/10.1016/j.jhazmat.2008.02.089>

Yu, Q., Zhang, Y., Wang, X., Ma, W. C., & Chen, L. M. (2009). Safety distance
assessment of industrial toxic releases based on frequency and consequence:
A case study in Shanghai, China. *J Hazard Mater*, 168(2–3), 955-961. doi:
<http://dx.doi.org/10.1016/j.jhazmat.2009.02.123>